Multiple Coulomb Scattering Methods in LAHET3$^{\text{TM}}$ and MCNPX$^{\text{TM}}$

Summary

The algorithms for charged particle tracking with multiple Coulomb scattering are documented for both LAHET3[1] and MCNPX[2]. The origin and computation of the required material-dependent scattering parameters are given, and recommendations for future code development are outlined.

I. Introduction

For charged particle tracking in LAHET3 and MCNPX, the simulation of the collective effect of multiple Coulomb scattering is applied over a small tracking step Δ. To outline the algorithm, we assume at the start of one step, the particle is directed in the +z-direction with direction vector $\vec{\Omega_0} = (0, 0, 1)$ and position $\vec{R_0} = (0, 0, 0)$. Applying the sampling algorithm, at the end of the step the direction is

$$\vec{\Omega} = (\theta_x, \theta_y, \sqrt{1 - \theta_x^2 - \theta_y^2})$$

and position is

$$\vec{R} = (\delta_x, \delta_y, \sqrt{\Delta^2 - \delta_x^2 - \delta_y^2})$$

where $\sqrt{\theta_x^2 + \theta_y^2} \ll 1$ and $\sqrt{\delta_x^2 + \delta_y^2} \ll \Delta$.

Following Rossi[3], it is assumed that, for sufficiently small step size, the quantities $\theta_x, \theta_y, \delta_x$ and δ_y may be sampled from Gaussian distributions with mean zero and variance dependent on the material in which the step occurs. Rotational invariance in the medium assures statistical independence of the x- and y- directions. In the following, the sampling/tracking algorithms are discussed and the material-dependent parameters needed are defined.

II. The LAHET Sampling Algorithm

Starting from Rossi's equation 2.17.6, the joint probability distribution for δ_x and θ_x is given by

$$P(\theta_x, \delta_x) = P(\theta_x \mid \delta_x)P(\delta_x) = \frac{\sqrt{3}}{4\pi\sigma_0^2\Delta} \exp\left(-\frac{\theta_x^2 - 3\delta_x\theta_x/\Delta + 3\delta_x^2/\Delta^2}{2\sigma_0^2}\right) \tag{1}$$

provided that we identify $\sigma_0^2 = \Theta_s^2 x/8$ and $\rho\Delta = x$, where ρ is the gram-density and x is in gm/cm^2. The LAHET sampling scheme is equivalent to sampling δ_x from the distribution

$$P(\delta_x) = \frac{\sqrt{3}}{2\sqrt{2\pi}\sigma_0\Delta} \exp\left(-\frac{3\delta_x^2}{8\sigma_0^2\Delta^2}\right) \tag{2}$$

and then sampling θ_x from the *conditional* probability distribution

$$P(\theta_x \mid \delta_x) = \frac{1}{\sqrt{2\pi}\sigma_0} \exp\left(-\frac{(\theta_x - 3\delta_x/2\Delta)^2}{2\sigma_0^2}\right) \tag{3}$$

The same equations apply for sampling θ_y and δ_y.

An alternative scheme, used with Gaussian scattering in other codes including GEANT, is to sample θ_x first from

$$P(\theta_x) = \frac{1}{2\sqrt{2\pi}\sigma_0} \exp\left(-\frac{\theta_x^2}{8\sigma_0^2}\right) \tag{4}$$

and *then* to sample δ_x from the conditional distribution

$$P(\delta_x \mid \theta_x) = \frac{\sqrt{3}}{\sqrt{2\pi}\sigma_0\Delta} \exp\left(-\frac{3(\delta_x - \Delta\theta_x/2)^2}{2\sigma_0^2\Delta^2}\right) \tag{5}$$

From equation (4), we obtain the important relationship for the mean square scattering angle

$$\langle\Theta^2\rangle = \langle\theta_x^2 + \theta_y^2\rangle = 2\langle\theta_x^2\rangle = 2\langle\theta_y^2\rangle = 8\sigma_0^2 \tag{6}$$

which illustrates that only one parameter $\langle\Theta^2\rangle$ (or σ_0) need be provided for the sampling algorithm.

The above equations also illustrate how a "transverse-lateral correction" (TLC) is applied in LAHET. The execution of a single step implies a small positional displacement as well as a small deflection in angle. It permits simulation of the spatial dispersion of a narrow beam with fewer and larger steps than is possible if only an angular deflection, using equation (4), is applied on each step.

For a given predetermined substep length Δ, which may also be determined by an interaction point, the distance to an intervening intersection with a surface $\Delta' < \Delta$ is calculated as the

straight-line distance to the surface along the *vector* from the beginning to the end of the substep. The particle is translated to the intersection point and the direction cosines for the particle are calculated using the new Δ'. Consequently, very small errors are introduced in the displacement, since the straightline distance is used, and in the angular deflection, since Δ' is not exactly the path length to the intersection point.

III. The MCNPX Sampling Algorithm

In MCNPX, the spatial displacement is applied as an undeflected translation of step size Δ in the initial $\vec{\Omega}_0$ direction. At the end of the step, which may have been truncated by an intervening surface as discussed above, the angular deflection is obtained through a modification of the sampling scheme implied by equation (4). Since equation (5) not needed, using equation (4) for both θ_x and θ_y along with the coordinate transformations $\Theta^2 = \theta_x^2 + \theta_2^2$, $\theta_x = \Theta \cos \phi$ and $\theta_y = \Theta \sin \phi$ allows Θ^2 to be sampled directly from

$$P(\Theta^2) = \frac{1}{8\sigma_0^2} \exp\left(-\frac{\Theta^2}{8\sigma_0^2}\right) = \frac{1}{\langle\Theta^2\rangle} \exp\left(-\frac{\Theta^2}{\langle\Theta^2\rangle}\right)$$

along with a uniform sampling of azimuthal angle ϕ.

Note that although MCNPX does not use the TLC described above, Δ is computed as an MCNPX "substep" which is generally smaller and frequently *much* smaller than the default step size applied in LAHET3. It is doubtful that any significant difference could be observed except in the spatial distribution of a narrow beam exiting a foil of only a few substeps in thickness.

IV. The Mean-square Deflection Angle $\langle\Theta^2\rangle$

The computation of $\langle\Theta^2\rangle$ follows Rossi[3]. The derivation is included here for the benefit of those who may wish to modify the current codes. Make the following definitions:

electron mass m_e (MeV/c^2)

"conventional electron radius" $r_e = e^2/m_e c^2$ (cm)

Rossi's nuclear radius parameter $r_0 = 0.49 r_e$

fine-structure constant α

Avogadro's number N_A

atom density of material N $(\text{barn-cm})^{-1}$

isotopic fraction f_i $(\sum f_i = 1)$

isotopic atom density $n_i = f_i N$ $(\text{barn-cm})^{-1}$

isotopic charge Z_i

isotopic mass number A_i

isotopic weight W_i

mean atomic weight of material $\bar{A} = \sum_j f_j W_j$

mass fraction $w_i = f_i W_i / \bar{A}$

mass density $\rho = \sum_j n_j W_j / (10^{-24} N_A) = N\bar{A}/(10^{-24} N_A)$ (gm/cm^3)

isotopic mass density $\rho_i = w_i \rho = N f_i W_i / (10^{-24} N_A)$ (gm/cm^3)

step size Δ (cm)

step size $x = \rho\Delta$ (grams/cm^2)

projectile charge Z_p

projectile mass M_p (MeV/c^2)

projectile kinetic energy K (MeV)

projectile momentum p (MeV/c)

For Z_p and any one isotope i in a mixture, Rossi's equations 2.16.3 and 2.16.8 provide

$$\langle \Theta_i^2 \rangle = 8\pi r_e^2 Z_p^2 \Delta \left(\frac{m_e c}{\beta p} \right)^2 \frac{N_A \rho_i}{W_i} Z_i(Z_i + 1) \ln \frac{\Theta_2}{\Theta_1} \tag{7}$$

where $Z_i(Z_i + 1)$ has been substituted for Z_i^2. Rossi's equation 2.15.12 is used for the small angle cutoff Θ_1 (representing nuclear screening)

$$\Theta_1 = \alpha Z_i^{1/3} \frac{m_e c}{p}$$

and equation 2.15.14 for the large angle cutoff (representing finite nuclear size)

$$\Theta_2 = \frac{\hbar}{r_0 A_i^{1/3} p} = \frac{r_e}{r_0} \frac{m_e c}{\alpha p A_i^{1/3}}$$

Using $\rho_i = f_i N W_i / 10^{-24} N_A$ and summing over the isotopes in the material, we obtain

$$\langle \Theta^2 \rangle = 8\pi r_e^2 Z_p^2 N \Delta \left(\frac{m_e c}{\beta p} \right)^2 10^{+24} \sum_i f_i Z_i(Z_i + 1) \ln \frac{r_e}{r_0 \alpha^2 A_i^{1/3} Z_i^{1/3}} \tag{8}$$

The variable in the codes which is computed during the initial stage, for each material, is

$$S = \sqrt{\pi} r_e m_e c^2 \left(10^{+24} N \sum_i f_i Z_i(Z_i + 1) \ln \frac{r_e}{r_0 \alpha^2 A_i^{1/3} Z_i^{1/3}} \right)^{1/2} \tag{9}$$

Following Rossi, we may write

$$\langle \Theta^2 \rangle = \frac{4\pi}{\alpha} \left(\frac{m_e c^2}{\beta c p} \right)^2 Z_p^2 \frac{x}{X_0} \tag{10}$$

and obtain the equivalent radiation length X_0 in this formulation as

$$\begin{aligned} \frac{1}{X_0} &= \frac{4\alpha r_e^2 N_A}{\bar{A}} \sum_i f_i Z_i (Z_i + 1) \ln \frac{(r_e/r_0)^{1/2}}{\alpha A_i^{1/6} Z_i^{1/6}} \\ &= \frac{4\alpha r_e^2 N_A}{\bar{A}} \sum_i f_i Z_i (Z_i + 1) \ln \frac{195.77}{A_i^{1/6} Z_i^{1/6}} \end{aligned} \tag{11}$$

where $\bar{A} = \sum_j f_j W_j$. The quantity S is then

$$S = m_e c^2 \left(\frac{\pi}{2\alpha} \frac{\rho}{X_0} \right)^{1/2} = 7.5 \text{MeV} \left(\frac{\rho}{X_0} \right)^{1/2}$$

V. Comparison with Conventional Methods

From equation (10), we get

$$\theta_0 = \sqrt{\langle \Theta^2 \rangle / 2} = \frac{15 \text{MeV}}{\beta c p} Z_p \sqrt{x/X_0} \tag{12}$$

with X_0 given by equation (11). The above form was commonly used at the time of time of the development of the original HETC[4] code and was continued in the development of LAHET[5].

Highland's formula[6], as modified by Lynch and Dahl[7], is conventionally written as

$$\theta_0 = \frac{13.6 \text{MeV}}{\beta c p} Z_p \sqrt{x/X_0} \left[1 + 0.038 \ln(x/X_0) \right] \tag{13}$$

with X_0 given by Tsai[8]. The ratio of X_0 from equation (11) to Tsai's value is shown in figure 1; the differences are less that 10%. The ratio of the mean deflection angle from (12) to the value calculated from (13) **at** $x = X_0$ is shown in figure 2. For the stated condition, $x = X_0$, the RMS deflection angle will be 7.5% to 15% larger with the current model than computed using Lynch and Dahl.

Note that

$$0.74 < 1 + 0.038 \ln(x/X_0) < 1.17 \tag{14}$$

over the prescribed range of validity $10^{-3} < x/X_0 < 100$. Thus the deviation is much greater than shown in figure 2 for regions much thinner or thicker than one radiation length.

VI. Recommendations

Two possibilities are easy to implement. First, the use of Tsai's[8] formulation for the radiation length may be made an input option. Second, the overall factor in equation (12) may be defined by user input.

However, dealing with the logarithmic factor in (14) is a great complication with the current tracking algorithms. As long as $\langle \Theta^2 \rangle \propto \Delta$ (or x), the cumulative deflection across a region is largely independent of the size and number of the steps taken at which the multiple scattering algorithm is applied, provided the energy loss in each step is sufficiently small. Such steps may be introduced by surfaces embedded in or between materials. Applying (13) with x defined on each step can produce significant differences, for example, between describing a region as a "packet" of many very thin foils or as a single unit, even though the areal density is the same.

The following are some options that could be introduced without altering the existing tracking in the codes.

- Allow the factor $1 + 0.038 \ln(x/X_0)$ to be applied on each multiple scattering step (with warning to user).

- Allow the logarithmic factor to be specified with a constant multiple of the radiation length over the system: $\ln(x/X_0) = \ln(cX_0/X_0) = \ln c$, which could be absorbed into the overall constant.

- Allow the logarithmic factor to be specified with a characteristic length parameter ℓ (in cm) over the system: $\ln(x/X_0) = \ln(\rho\ell/X_0)$, which is a constant within each material.

- Allow an arbitrary specification by material or by cell.

Although none of the above is ideal, each would provide some flexibility for dealing with different classes of calculations.

REFERENCES

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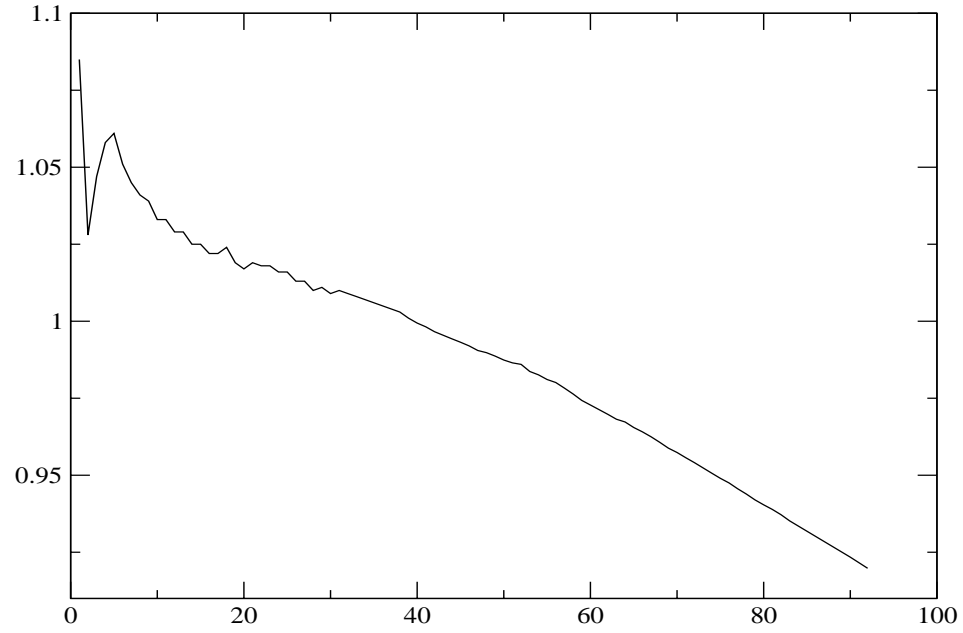
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Figure 1: Ratio of the radiation length calculated from equation (11) to the radiation length from Tsai's formula.
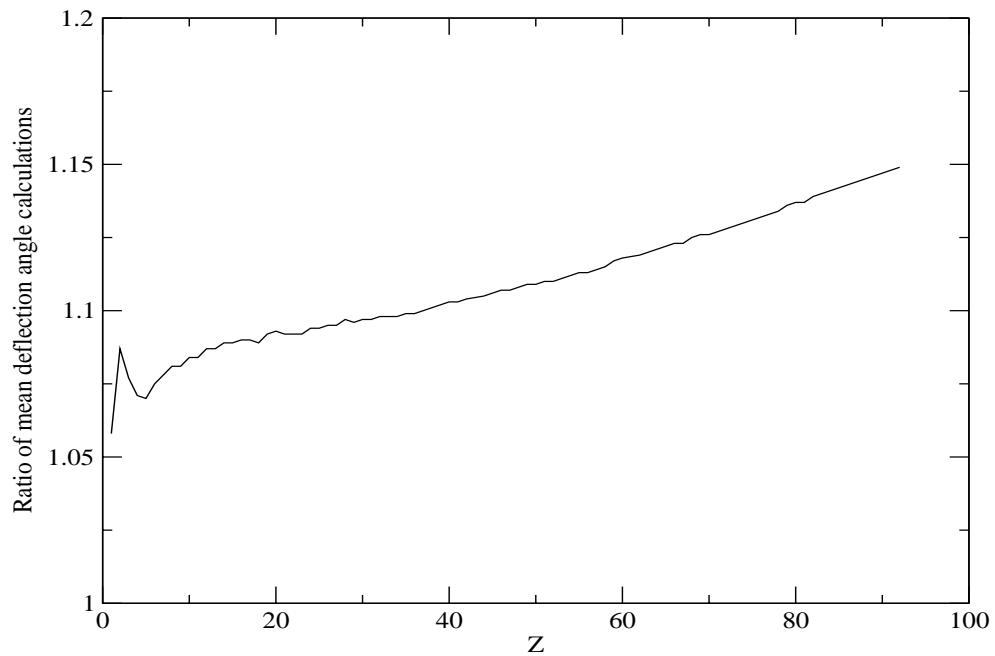

Figure 2: Ratio of the mean deflection angle from equation (12) to the value calculated from equation (13) at $x = X_0$